EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 15 —

http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2014/

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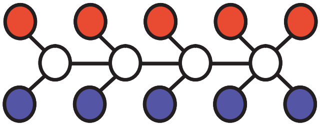
Nov 19th, 2014



Announcements

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* `http://www.nowpublishers.com/product.aspx?product=MAL&doi=2200000001`
- Read chapters 1,2, and 3 in this book. Start reading chapter 4.
- Assignment due Friday (Nov 21st) morning, 9:am. Final project proposals (one page max).

Class Road Map - EE512a

- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, elimination, Inference on Trees
- L3 (10/6): Tree inference, message passing, more general queries, non-tree)
- L4 (10/8): Non-trees, perfect elimination, triangulated graphs
- L5 (10/13): triangulated graphs, k-trees, the triangulation process/heuristics
- L6 (10/15): multiple queries, decomposable models, junction trees
- L7 (10/20): junction trees, begin intersection graphs
- L8 (10/22): intersection graphs, inference on junction trees
- L9 (10/27): inference on junction trees, semirings,
- L10 (11/3): conditioning, hardness, LBP
- L11 (11/5): LBP, exponential models,
- L12 (11/10): exponential models, mean params and polytopes,
- L13 (11/12): polytopes, tree outer bound, Bethe entropy approx.
- L14 (11/17): Bethe entropy approx, loop series correction
- L15 (11/19): Hypergraphs, posets, Mobius, Kikuchi
- L16 (11/24):
- L17 (11/26):
- L18 (12/1):
- L19 (12/3):
- Final Presentations: (12/10):

Finals Week: Dec 8th-12th, 2014.

Bethe Variational Problem and LBP

Original variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\} \tag{15.14}$$

Approximate variational representation of log partition function

$$A_{\text{Bethe}}(\theta) = \sup_{\tau \in \mathbb{L}} \{\langle \theta, \tau \rangle + H_{\text{Bethe}}(\tau)\} \tag{15.15}$$

$$= \sup_{\tau \in \mathbb{L}} \left\{ \langle \theta, \tau \rangle + \sum_{v \in V(G)} H_v(\tau_v) - \sum_{(s,t) \in E(G)} I_{st}(\tau_{st}) \right\} \tag{15.16}$$

- Exact when $G = T$ but we do this for any G, still commutable
- we get an approximate log partition function, and approximate (pseudo) marginals (in $\mathbb{L}$), but this is perhaps much easier to compute.
- We can optimize this directly using a Lagrangian formulation.

Comparison of A and A_{Bethe}: loop series expansion

Proposition 15.2.2

Consider a pairwise MRF with binary variables, with $A_{Bethe}(\theta)$ being the optimized free energy evaluated at a LBP fixed point $\tau = (\tau_s, s \in V; \tau_{st}, (s,t) \in E(G))$. Then we have the following relationship with the cumulant function $A(\theta)$.

$$A(\theta) = A_{Bethe}(\theta) + \log \left\{ 1 + \sum_{\emptyset \neq \tilde{E} \subseteq E} \beta_{\tilde{E}} \prod_{s \in V} \mathbb{E}_{\tau_s} \left[(X_s - \tau_s)^{d_s(\tilde{E})} \right] \right\} \quad (15.6)$$

- For any $\tilde{E}$ such that $\exists s$ with $d_s(\tilde{E}) = 1$, inner term is zero and vanishes. why? Since $E_{\tau_s}\left[(X_s - \tau_s)^d\right]$ is the d^{th} central moment. Thus, terms in the sum only exists for generalized loops.
- The generalized loops give the correction!
- For trees, there are no generalized loops, and so if G is a tree then we have an equality between $A(\theta)$ and $A_{\text{Bethe}}(\theta)$ (recall both defs here).

General idea of Kikuchi

- Variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathbb{M}(G)} \{\langle \theta, \mu \rangle - A^*(\mu)\} \tag{15.14}$$

- So far, we used a replacement for $-A^*(\mu)$ and $\mathbb{M}(G)$ inspired by trees.
- A tree is just a 1-tree, so one simple generalization would be to use a k-tree, for constant k, where k is not too large.
- More generally still, why not some other structure, like junction tree (embedable into a k-tree for k not too large).
- Junction trees are hypertrees (to be defined) that satisfy r.i.p. (special case of hypergraphs). Every clique need not be of size $k+1$.
- So approach is the following: 1) derive expression for $-A^*(\mu)$ associated with a hypertree/junction tree; 2) generalize this expression for any hypergraph; 3) consider local consistency properties of hypertrees/junction tree; 4) use hypertrees local consistency property for generalized polytope associated with any hypergraph.
- $\Rightarrow$ Kikuchi variational approach ("clustered variational approximation")

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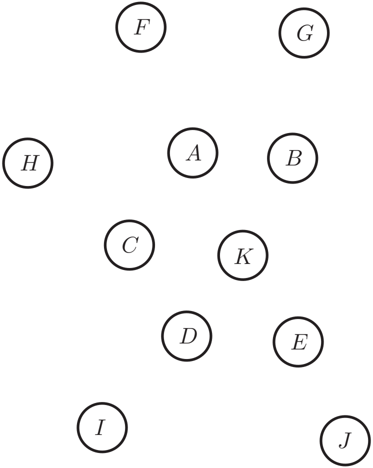
- In a graph, $|e| = 2$. Thus, a graph is a (restricted) hypergraph, but not vice verse.

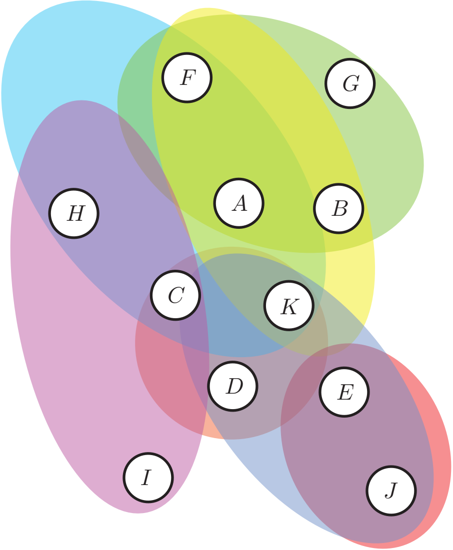
Drawing/Visualizing Hypergraphs

- A set of vertices, normally edges connect two nodes.



Drawing/Visualizing Hypergraphs

- Hypergraph: hyperedges are shaded regions, each region a vertex cluster



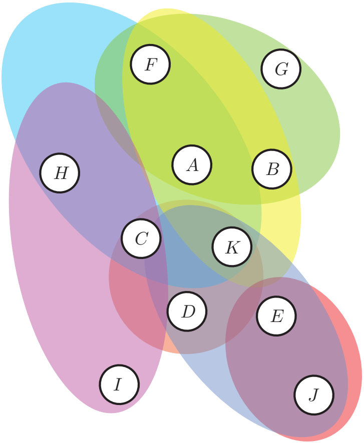
Hypergraphs and bipartite graphs

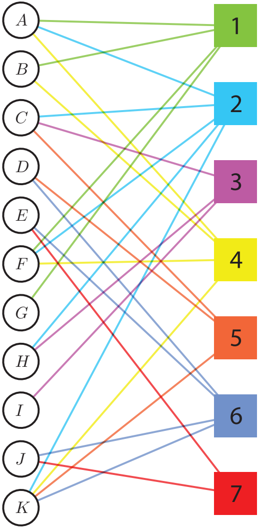
Hypergraphs can be represented by a bipartite $G = (V, F, E)$ graphs where V is a set of left-nodes, F is a set of right nodes, and E is a set of size-two edges. Right nodes are hyperedges in the hypergraphs.

Next slide shows an example.

Drawing/Visualizing Hypergraphs as Bipartite Graphs

- Hypergraph (shaded regions) on left, while bipartite graph representation on the right.





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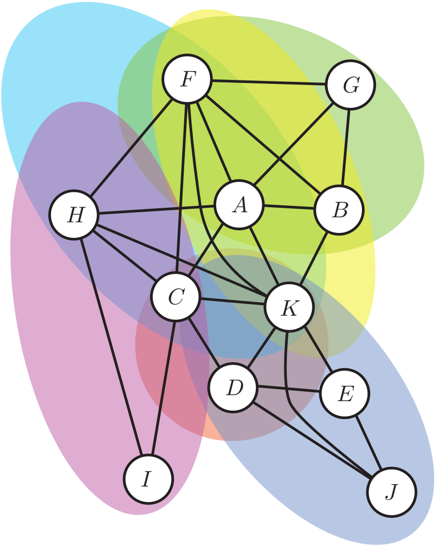
- A hypergraph H is acyclic if H is conformal and $G(H)$ is chordal/triangulated.

Drawing/Visualizing Hypergraphs

- Shaded regions are cluster edge cover of "conformal" graph



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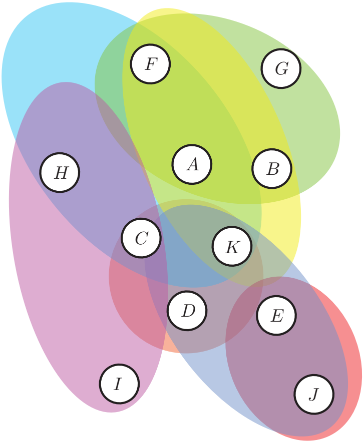

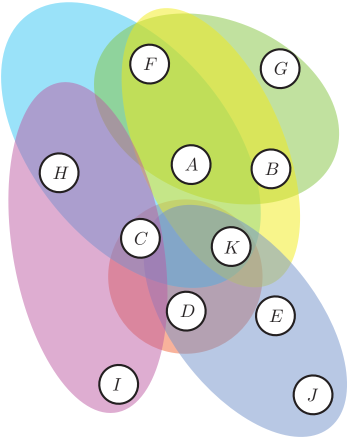

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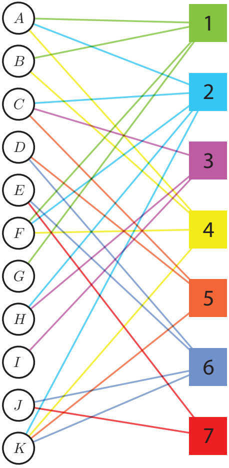

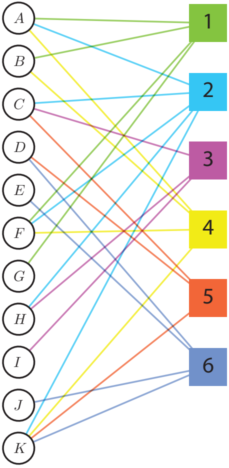

Hypergraphs and Junction Trees

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- In fact, a junction tree is a hypertree where the cliques (which are clusters of original graph nodes) in the junction tree are the edges of the hypertree.

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Definition 15.3.5 (hypertree)

A hypergraph H that is acyclic is called a *hypertree*.

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For all $x, x \preceq x$.	(Reflexive)	(P1.)
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- We can use the above to get other operators as well such as "less than" via $x \preceq y$ and $x \neq y$ implies $x \prec y$. And $x \succeq y$ is read "x contains y". And so on.

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- The length of a chain of n elements is $n - 1$.

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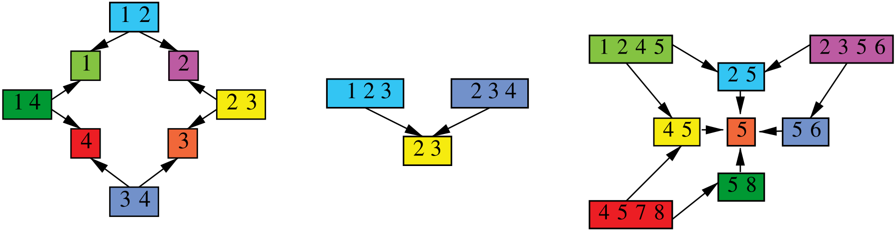

(a) (b) (c)

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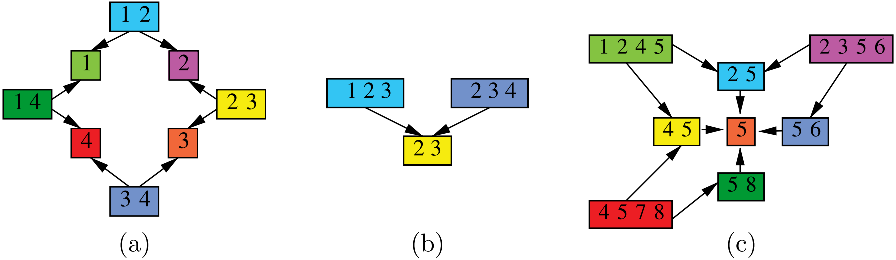
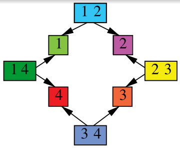


- Which ones, if any, are in reduced representation?

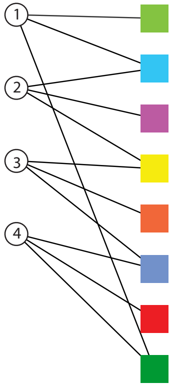
Hypergraph, edge representations, bipartite graphs



(a)

Edge-representations of hypergraphs and their corresponding bipartite graph representation.

An ordinary single 4-cycle graph represented as a hypergraph.



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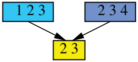
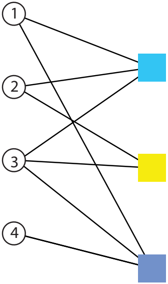
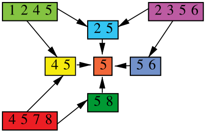


(b)



Edge-representations of hypergraphs and their corresponding bipartite graph representation.
A simple hypertree of "width" two.

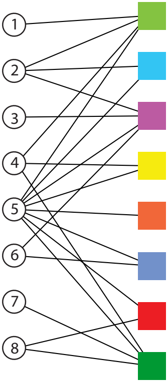
Hypergraph, edge representations, bipartite graphs



(c)

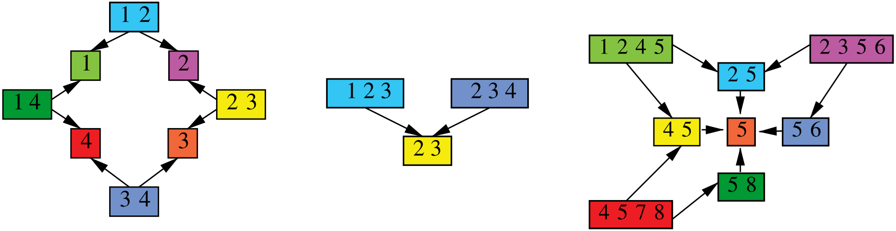
Edge-representations of hypergraphs and their corresponding bipartite graph representation.

A more complex hypertree of "width" three.



Hypergraph, edge representations, and posets

- Hypergraphs and edge representations.



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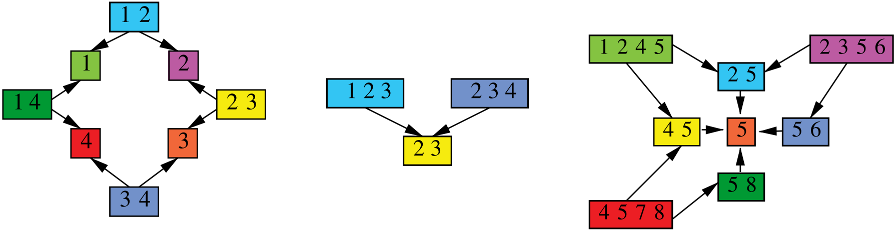

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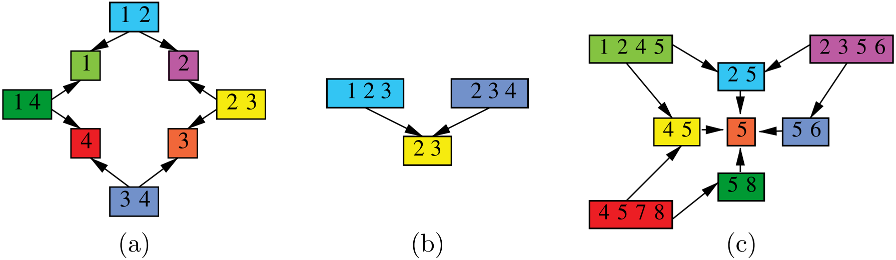

- Here, $a \to b$ if it is the case that $b \preceq a$ and there does not exist a c such that $b \preceq c \preceq a$, similar to a Hasse lattice diagram.
- Hence, the edges of a hypergraph form a partially ordered set.

Inclusion-Exclusion

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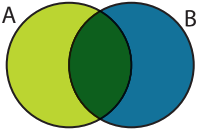

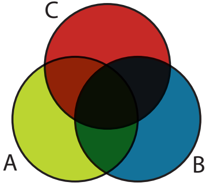

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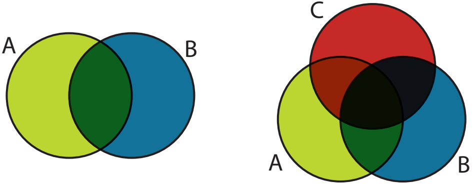

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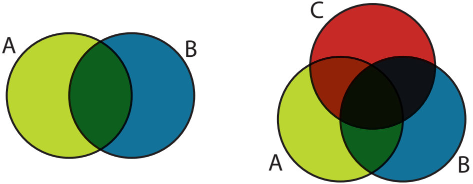

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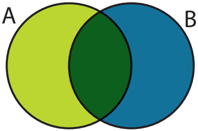

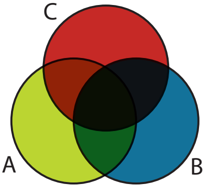

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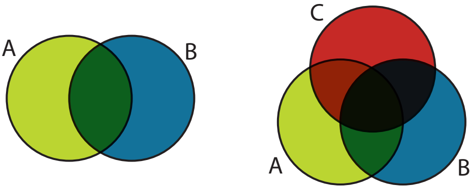

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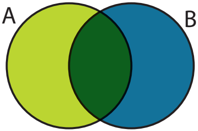

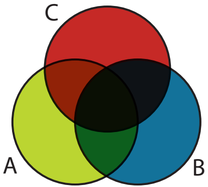

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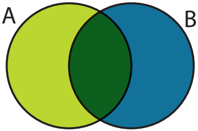

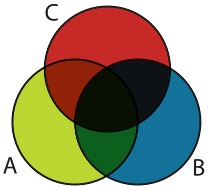

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Entropic Inclusion-Exclusion

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- That is, we have

$$
\begin{aligned}
H(X,Y) &= H(X) + H(Y) - I(X;Y) && (15.1)\\
H(X,Y,Z) &= H(X) + H(Y) + H(Z) && (15.2)\\
&\quad - I(X;Y) - I(X;Z) - I(Y;Z) && (15.3)\\
&\quad + I(X;Y;Z). && (15.4)
\end{aligned}
$$

and so on (see Yeung's book on information theory, the chapter on information measures).

Inclusion/Exclusion, general form for set measure

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Inclusion/Exclusion, general form for set measure

- Given $X_1, X_2, \ldots, X_n \subseteq U$,
- Exclusion/exclusion formula for cardinality set measure $\mu(X) = |X|$:

$$\mu(\cap_{i=1}^n X_i) = \sum_{i=1}^n \mu(X_i) - \sum_{1 \leq i < j \leq n} \mu(X_i \cup X_j) \tag{15.5}$$

$$+ \sum_{1 \leq i < j < k \leq n} \mu(X_i \cup X_j \cup X_k) + \ldots \tag{15.6}$$

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- A "dual" form has the form:

$$\mu(\cup_{i=1}^n X_i) = \sum_{i=1}^n \mu(X_i) - \sum_{1 \le i < j \le n} \mu(X_i \cap X_j) \tag{15.8}$$

$$+ \sum_{1 \le i < j < k \le n} \mu(X_i \cap X_j \cap X_k) + \ldots \tag{15.9}$$

$$+ (-1)^{n-1} \mu(X_1 \cap X_2 \cap \ldots \cap X_n) \tag{15.10}$$

Inclusion/Exclusion, general form for set measure

- Another (easier, shorter) way of writing these is as:

$$\mu(\cap_{i=1}^n X_i) = \sum_{k=1}^n (-1)^{k+1} \left(\sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} \mu(X_{i_1} \cup \cdots \cup X_{i_k}) \right) \tag{15.11}$$

and

$$\mu(\cup_{i=1}^n X_i) = \sum_{k=1}^n (-1)^{k+1} \left(\sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} \mu(X_{i_1} \cap \cdots \cap X_{i_k}) \right) \tag{15.12}$$

Möbius Inversion Lemma and Inclusion-Exclusion

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$$\forall A \subseteq V : \Upsilon(A) = \sum_{B : B \subseteq A} \Omega(B) \tag{15.13}$$

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- We use it here to come up with alternative expressions for the entropy and for the marginal polytope.

Hammersley Clifford Theorem

Theorem 15.3.6

(Hammersley and Clifford) Let $\mathcal{F}^+$ be the family of distributions with positive (and continuous in the continuous case) density (i.e., $p(x) > 0$ for all $p \in \mathcal{F}^+$). Then $\mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M}^{(f)}) = \mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M}^{(p)})$.

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- $\mathcal{F}(G, \mathcal{M}^{(p)})$ refers to the pairwise Markov property which states that if $u, v \in V(G)$ are not connected by an edge, then $X_u \perp\!\!\!\perp X_v \perp\!\!\!\perp X_{V \setminus \{u,v\}}$.

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- In fact, $\mathcal{F}(G, \mathcal{M}^{(p)}) \supseteq \mathcal{F}(G, \mathcal{M}^{(f)})$. always holds. Hammersley and Clifford theorem (which uses Möbius inversion lemma) shows that $\mathcal{F}^+(G, R^{(p)}) \subseteq \mathcal{F}^+(G, R^{(f)})$, where $\mathcal{F}^+(G, \mathcal{M}) = \mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M})$.

Möbius Inversion Lemma

Lemma 15.3.7 (Möbius Inversion Lemma (for sets))

Let Υ and Ω be functions defined on the set of all subsets of a finite set V, taking values in an Abelian group (i.e., a set and an operator having properties closure, associativity, identity, and inverse, and for which the elements also commute, the real numbers being just one example). The following two equations imply each other.

$$\forall A \subseteq V : \Upsilon(A) = \sum_{B : B \subseteq A} \Omega(B) \tag{15.15}$$

$$\forall B \subseteq V : \Omega(B) = \sum_{C : C \subseteq B} (-1)^{|B \setminus C|} \Upsilon(C) \tag{15.16}$$

Proof of Möbius Inversion Lemma

Proof.

$$\sum_{B:B\subseteq A} \Omega(B) = \sum_{B:B\subseteq A} \sum_{C:C\subseteq B} (-1)^{|B\setminus C|} \Upsilon(C) \tag{15.17}$$

$$= \sum_{C:C\subseteq A} \sum_{B:C\subseteq B \& B\subseteq A} \Upsilon(C)(-1)^{|B\setminus C|} \tag{15.18}$$

$$= \sum_{C:C\subseteq A} \Upsilon(C) \sum_{B:C\subseteq B \& B\subseteq A} (-1)^{|B\setminus C|} \tag{15.19}$$

$$= \sum_{C:C\subseteq A} \Upsilon(C) \sum_{H:H\subseteq A\setminus C} (-1)^{|H|} \tag{15.20}$$

Proof of Möbius Inversion Lemma

Proof Cont.

Also, note that for any set D,

$$\sum_{H:H\subseteq D} (-1)^{|H|} = \sum_{i=0}^{|D|} \binom{|D|}{i} (-1)^i = \sum_{i=0}^{|D|} \binom{|D|}{i} (-1)^i (1)^{|D|-i} \tag{15.21}$$

$$= (1-1)^{|D|} = \begin{cases} 1 & \text{if } |D| = 0 \\ 0 & \text{otherwise} \end{cases} \tag{15.22}$$

which means that when we take $D = A \setminus C$, with $C \subseteq A$, we get

$$\sum_{H:H\subseteq A\setminus C} (-1)^{|H|} = \begin{cases} 1 & \text{if } A = C \\ 0 & \text{otherwise} \end{cases} \tag{15.23}$$

Proof of Möbius Inversion Lemma

Proof Cont.

This gives

$$\sum_{B:B\subseteq A} \Omega(B) = \sum_{C:C\subseteq A} \Upsilon(C)\mathbf{1}\{A = C\} = \Upsilon(A) \tag{15.24}$$

thus proving one direction. The other direction is very similar. □

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- Let $\mathcal{P}$ be a partially ordered set with binary relation $\preceq$.
- A zeta function of a poset is a mapping $\zeta : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ defined by

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- Given $\omega(g,f)$ defined for f such that $g \preceq f \prec h$, we define

$$\omega(g,h) = - \sum_{\{f | g \preceq f \prec h\}} \omega(g,f) \tag{15.26}$$

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$$\omega(g,h) = - \sum_{\{f | g \preceq f \prec h\}} \omega(g,f) \tag{15.26}$$

- Then, ω and ζ are multiplicative inverses, in that

$$\sum_{f \in \mathcal{P}} \omega(g,f)\zeta(f,h) = \sum_{\{f | g \preceq f \preceq h\}} \omega(g,f) = \delta(g,h) \tag{15.27}$$

General Möbius Inversion Lemma

Lemma 15.3.8 (General Möbius Inversion Lemma)

Given real valued functions Υ and Ω defined on poset $\mathcal{P}$, then $\Omega(h)$ may be expressed via $\Upsilon(\cdot)$ via

$$\Omega(h) = \sum_{g \preceq h} \Upsilon(g) \quad \textit{for all } h \in \mathcal{P} \tag{15.28}$$

iff $\Upsilon(h)$ may be expressed via $\Omega(\cdot)$ via

$$\Upsilon(h) = \sum_{g \preceq h} \Omega(g)\omega(g, h) \quad \textit{for all } h \in \mathcal{P} \tag{15.29}$$

When $\mathcal{P} = 2^V$ for some set V (so this means that the poset consists of sets and all subsets of an underlying set V) this can be simplified, where $\preceq$ becomes $\subseteq$; and $\succeq$ becomes $\supseteq$, like we saw above.
(see Stanley, "Enumerative Combinatorics" for more info.)

Back to Kikuchi: Möbius and expressions of factorization

- Suppose we are given marginals that factor w.r.t. a hypergraph $G = (V, E)$, so we have $\mu = (\mu_h, h \in E)$, then we can define new functions $\varphi = (\varphi_h, h \in E)$ via Möbius inversion lemma as follows

$$\log \varphi_h(x_h) \triangleq \sum_{g \preceq h} \omega(g, h) \log \mu_g(x_g) \tag{15.30}$$

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- Key, when φ_h is defined as above, and G is a hypertree we have

$$p_\mu(x) = \prod_{h \in E} \varphi_h(x_h) \tag{15.32}$$

$\Rightarrow$ general way to factorize a distribution that factors w.r.t. a hypergraph.

1-Tree factorization and Möbius

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- In such case, from Equation (15.31), we have that for all $s \in V$, $\varphi_s(x_s) = \mu_s(x_s)$ and for all $(s, v) = e \in E$, we have:

$$\varphi_{st}(x_s, x_t) = \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)} \tag{15.33}$$

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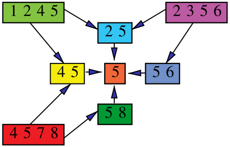
- Gives us the tree factorization we saw early in this course, namely:

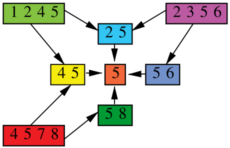
$$p(x) = \prod_{h \in E} \varphi_h(x_h) = \prod_{s \in V} \mu_s(x_s) \prod_{(s,t)=e \in E} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)} \tag{15.34}$$

HyperTree factorization and Möbius

- For the more general hyper-tree, consider edge set $E = \{(12345), (2356), (4578), (25), (45), (56), (58), (5)\}$. Check: is this a junction tree of cliques?



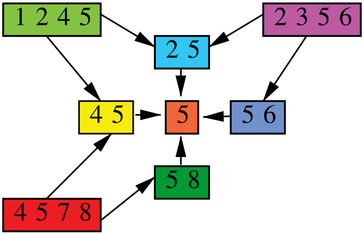
HyperTree factorization and Möbius



- For the more general hyper-tree, consider edge set $E = \{(12345), (2356), (4578), (25), (45), (56), (58), (5)\}$. Check: is this a junction tree of cliques?
- Then, from Eqn. (15.31), we get unaries $\varphi_s(x_s) = \mu_s(x_s)$ and pairwise (e.g., $\varphi_{25} = \mu_{25}/\mu_5$, etc.) and

$$\varphi_{1245} = \frac{\mu_{1245}}{\varphi_{25}\varphi_{45}\varphi_5} = \frac{\mu_{1245}}{\frac{\mu_{25}}{\mu_5}\frac{\mu_{45}}{\mu_5}\mu_5} = \frac{\mu_{1245}\mu_5}{\mu_{25}\mu_{45}} \tag{15.35}$$

expressions of factorization and Möbius

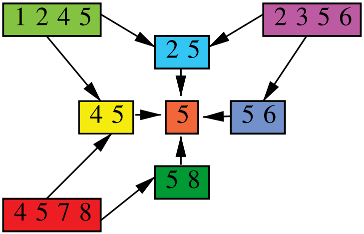


- Doing this for all maxcliques of the figure, we get a factorization of the form:

$$p_\mu = \frac{\mu_{1245}\mu_5}{\mu_{25}\mu_{45}} \frac{\mu_{2356}\mu_5}{\mu_{25}\mu_{56}} \frac{\mu_{4578}\mu_5}{\mu_{45}\mu_{58}} \frac{\mu_{25}}{\mu_5} \frac{\mu_{45}}{\mu_5} \frac{\mu_{56}}{\mu_5} \frac{\mu_{58}}{\mu_5} \mu_5 \tag{15.36}$$

$$= \frac{\mu_{1245}\mu_{2356}\mu_{4578}}{\mu_{25}\mu_{45}} \tag{15.37}$$

expressions of factorization and Möbius



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- This is the same as the junction tree factorization with max cliques $\{1245\}$, $\{4578\}$, and $\{2356\}$ and separators $\{25\}$ and $\{45\}$.

New expressions of entropy

- Can express entropic quantities as well, such as the hyperedge entropy

$$H_h(\mu_h) = -\sum_{x_h} \mu_h(x_h) \log \mu_h(x_h) \tag{15.38}$$

and the "multi-information" function

$$I_h(\mu_h) = \sum_{x_h} \mu_h(x_h) \log \varphi_h(x_h) \tag{15.39}$$

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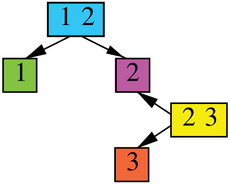
- In the case of a single tree edge $h = (s,t)$, then $I_h(\mu_h) = I(X_s; X_t)$ the standard mutual information $(= H(X_s) + H(X_t) - H(X_s, X_t))$.



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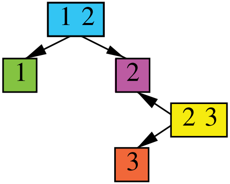

- By Eqn (15.32), overall entropy of any hypertree distribution becomes

$$H_{\text{hyper}}(\mu) = -\sum_{h \in E} I_h(\mu_h) \tag{15.40}$$

multi-information decomposition

- Using Möbius, and Eqn. (15.30) we can write

$$I_h(\mu_h) = \sum_{x_h} \mu_h(x_h) \log \varphi_h(x_h) = \sum_{x_h} \mu_h(x_h) \left(\sum_{g \preceq h} \omega(g,h) \log \mu_g(x_g) \right)$$

$$= \sum_{g \preceq h} \omega(g,h) \left\{ \sum_{x_h} \mu_h(x_h) \log \mu_g(x_g) \right\}$$

$$= \sum_{f \preceq h} \sum_{e \succeq f} \omega(f,e) \left\{ \sum_{x_f} \mu_f(x_f) \log \mu_f(x_f) \right\} = -\sum_{f \preceq h} c(f) H_f(\mu_f)$$

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where we define overcounting numbers ($\sim$ shattering coefficient)

$$c(f) \triangleq \sum_{e \succeq f} \omega(f,e) \tag{15.41}$$

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where we define overcounting numbers ($\sim$ shattering coefficient)

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- This gives us a new expression for the hypertree entropy

$$H_{\text{hyper}}(\mu) = \sum_{h \in E} c(h) H_h(\mu_h) \tag{15.42}$$

Usable to get Kikuchi variational approximation

- Given arbitrary hypergraph now, we can generalize the hypertree-specific expressions above to this arbitrary hypergraph. This will give us a variational expression that approximates cumulant.

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  using same form of parameterization.
- Hypergraph will give us local marginal constraints on hypergraph pseudo marginals, i.e., for each $h \in E$, we form marginal $\tau_h(x_h)$ and define constraints, non-negative, and

$$\sum_{x_h} \tau_h(x_h) = 1 \tag{15.44}$$

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- Sum to one constraint:

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- Define new polyhedral constraint set $\mathbb{L}_t(G)$

$$\mathbb{L}_t(G) = \{\tau \geq 0 | \text{ Equations (15.45) } \forall h, \text{ and (15.46) } \forall g \preceq h \text{ hold}\} \tag{15.47}$$

Kikuchi variational approximation

- Generalized approximate (app) entropy for the hypergraph:

$$H_{\text{app}} = \sum_{g \in E} c(g) H_g(\tau_g) \quad (15.48)$$

where H_g is hyperedge entropy and overcounting number defined by:

$$c(g) = \sum_{f \succeq g} \omega(g, f) \quad (15.49)$$

Sources for Today's Lecture

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* http://www.nowpublishers.com/product.aspx?product=MAL&doi=2200000001